Specific heat of the simple-cubic Ising model

Xiaomei Feng[1,2] and Henk W.J. Blöte[1,3]

[1]*Faculty of Applied Sciences, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands*

[2]*Nanjing University of Aeronautics and Astronautics, College of Materials Science and Technology, 29 Yudao St., 210016 Nanjing, P.R. China and*

[3]*Lorentz Institute, Leiden University, P.O. Box 9506, 2300 RA Leiden, The Netherlands**

(Dated: December 8, 2009)

Abstract

We provide an expression quantitatively describing the specific heat of the Ising model on the simple-cubic lattice in the critical region. This expression is based on finite-size scaling of numerical results obtained by means of a Monte Carlo method. It agrees satisfactorily with series expansions and with a set of experimental results. Our results include a determination of the universal amplitude ratio of the specific-heat divergences at both sides of the critical point.

PACS numbers: 05.50.+q, 64.60.Cn, 02.60.-x

*Electronic address: henk@lorentz.leidenuniv.nl

I. INTRODUCTION

Though real magnetic systems were supposed to be Heisenberg-like, the Ising model was originally introduced [1] as a simplified model of magnetic ordering, because its relative simplicity offers better possibilities for a theoretical analysis. In later years, it was found, however, that Ising-like magnetic systems do exist. This is because real systems consist of spins embedded in a crystal lattice, and the resulting anisotropy field due to the neighboring charges may lift the O(3) symmetry of an unperturbed spin. Depending on the character of the perturbation, the spin may have an 'easy axis' or an 'easy plane'. Here we consider the former case, which leads to Ising-like behavior.

In many cases, the perturbation is relatively small and the system will approximately behave Heisenberg-like, except near an ordering transition where the paramagnetic state transforms into a long-range ordered one. Near the transition, crossover [2, 3, 4] occurs to Ising-like behavior. The critical singularities are then described by the Ising set of critical exponents. In some other cases, the perturbation due to the crystal field is so strong that the magnetic spins assume a true Ising character. This situation occurs when the ionic angular momentum $\vec{S}$ is described by a spin quantum number $S > \frac{1}{2}$, and the crystal field lifts the degeneracy of the S_z eigenstates such that the $S_z = \pm S$ doublet is lowest in energy, with the higher levels so far away that they play no role, even in the presence of exchange interactions between neighboring spins. Then the low-lying doublet can be described by an effective spin-1/2 Ising Hamiltonian. This situation is known to occur for the Co^{2+} ion in a tetrahedral coordination. It occurs also for some rare-earth ions like Dy^{3+} and Yb^{3+} in a sufficiently strong crystal field, with the provision that here the magnetic moments are due to spin as well as orbital angular momentum, and should thus be denoted $\vec{J}$ instead of $\vec{S}$.

If such ions are embedded in a crystal structure for which theoretical predictions for the thermodynamical properties such as the specific heat exist, comparison with experiments may be possible [5, 6]. Such comparisons were made for dysprosium phosphate [6, 7] and for some alkali cobalt halides [8, 9]. These systems were found to behave, at least approximately, as the Ising models on the diamond lattice and the simple-cubic lattice respectively.

The best way to obtain theoretical results for the thermodynamic properties of these models would obviously be an exact solution, but this is known to be a very difficult problem. It is thus noteworthy that it was claimed recently by Zhang [10] that a conjectured exact

solution was found for the three-dimensional Ising model. However, Perk [11] and Wu et al. [12] pointed out that Zhang's result for the free energy and the underlying arguments are flawed. Here it may be added that Zhang's result for the critical point of the simple-cubic Ising models is not compatible with independent and mutually consistent numerical estimates [13, 14]. The difference with Zhang's result exceeds the estimated numerical accuracies [13, 14] by several orders of magnitude.

In the absence of an exact solution, one may still resort to approximations. At temperatures sufficiently far above and below the critical point, excellent approximations exist in the form of series expansion of the partition function or the free energy, such as given in Refs. 15 and 16 for the model on the simple-cubic lattice. In the critical region, the series of a finite length become inaccurate, and a method to extrapolate these series on the basis of a critical scaling assumption, such as used by Butera and Comi [17], is needed. In the case of Rb_3CoCl_5 (rubidium cobalt chloride) [9] the required theoretical prediction for the specific heat near criticality was also obtained this way. A similar analysis has been performed for the specific heat of $DyPO_4$ (dysprosium phosphate) [6, 7], which was instead compared with series expansions for the diamond lattice. However, these specific-heat analyses were conducted at a time that the value of the critical exponent α was not well known, for instance, α was set to zero in Ref. 9. Moreover, Wegner's correction to scaling [18] was not included.

In order to obtain accurate predictions for the heat capacity in the critical region, one may apply Monte Carlo simulations. Cluster simulation methods [19, 20], which strongly reduce critical slowing down, allow statistically accurate simulations in the critical region. Extrapolation of the finite-size simulation data to the thermodynamic limit is possible if the simulations cover a range of finite sizes exceeding the correlation length. Whereas this still excludes, as a result of the divergence of the correlation length, a narrow temperature range about the critical point, one may attempt to describe the extrapolated data by means of a scaling formula. The present work reports our efforts along this line for the case of the energy and the specific heat of the Ising model on the simple-cubic lattice.

In Sec. II we describe our Monte Carlo simulations, and the extrapolation to infinite system size. The derivation of scaling formulas for the energy and the specific heat, and the data analysis in terms of these formulas, are presented in Sec. III. Section IV discusses the numerical accuracies, provides comparisons with results from series expansions and with a set of experimental results, and ends with a few concluding remarks.

II. NUMERICAL TECHNIQUE

The reduced Hamiltonian (Hamiltonian divided by kT) of the Ising model is denoted

$$\mathcal{H}(K) = -K \sum_{\langle i,j \rangle} s_i s_j \tag{1}$$

where the indices i and j label nearest-neighbor lattice sites on the simple-cubic lattice. The sum is on all nearest-neighbor pairs, and the spins s_k can assume values ± 1. The coupling is defined by $K \equiv J/kT$ where J is minus the energy of a pair of parallel nearest-neighbor spins, k the Boltzmann constant, and T the temperature. The canonical reduced free energy density f is equal to

$$f = \frac{1}{N} \ln Z \,, \qquad Z = \sum_{\{S\}} e^{-\mathcal{H}(K)} \tag{2}$$

where Z is the partition function, N the number of spins, and the sum is on all spin configurations $\{S\}$. The energy E and the specific heat C per particle, as expressed in dimensionless units, follow from the derivatives of f to K:

$$\frac{E}{J} = \frac{E}{kTK} = -\frac{df}{dK} \,, \qquad \frac{C}{k} = K^2 \frac{d^2 f}{dK^2} \,. \tag{3}$$

A. Monte Carlo calculations

Substitution of Eqs. (2) and (1) in Eqs. (3) leads to

$$\frac{E}{J} = \frac{1}{NK} \langle \mathcal{H} \rangle \tag{4}$$

and

$$\frac{C}{k} = \frac{1}{N} (\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2) \,, \tag{5}$$

where the ensemble averages $\langle x \rangle$, which are defined as

$$\langle x \rangle \equiv \frac{1}{Z} \sum_{\{S\}} x e^{-\mathcal{H}(K)} \,, \tag{6}$$

can be sampled directly using importance sampling.

The simulations involved the sampling of the energy, as well as its square, for $L \times L \times L$ Ising systems on simple-cubic lattices, with periodic boundary conditions. The system sizes were chosen as powers of 2 in the range $4 \leq L \leq 128$, and in addition as $L = 6$ and 12.

About 10^7 samples were taken for $L \leq 16$, 2×10^6 for $L = 32$, 3×10^5 for $L = 64$, and 5×10^4 for $L = 128$. Each sample was preceded by a number or Wolff cluster steps and/or Metropolis sweeps, depending on the value of K in comparison with the critical coupling $K_c \approx 0.2216546$ [14]. For $K << K_c$, Wolff clusters tend to be very small and only Metropolis sweeps were applied, and for $K > K_c$ only Wolff cluster steps. In the intermediate range, a few Metropolis sweeps were supplemented with a number of Wolff cluster steps. The number of Wolff clusters was chosen roughly equal to the inverse of the relative Wolff cluster size. The coupling K was given some 50 different values chosen to cover a wide range about the critical point.

B. Extrapolation

The analysis of the numerical finite-size data was done on the basis of well-documented finite-size scaling methods [21]. For non-critical systems with sizes L exceeding the correlation length, the data for the energy should approximately behave as

$$E(K, L) = E(K, \infty) + a(K)e^{-L/\xi(K)} + \cdots \tag{7}$$

from which the extrapolated energy $E(K, \infty)$ was obtained by means of a least-squares analysis. A small-system-size cutoff was applied when necessary to obtain a satisfactory residual χ^2. This cutoff varied between $L = 6$ far away from the critical point, and $L = 32$ at a distance $|K - K_c| \approx 0.005$ from the critical point. No reliable extrapolations were obtained for $|K - K_c|$ less than a few times 10^{-3}, with the exception of $K = K_c$, where one expects that the finite-size-dependent energy converges as a power of L, which again enables extrapolation to $L = \infty$. Typical estimated accuracies of the extrapolated results for E/J are in the order of 10^{-5}.

The same extrapolation procedure was applied to the finite-size data for the specific heat with $|K - K_c| > 0.005$. Typical accuracies of the extrapolated results for C/k are estimated as at most a few times 10^{-4} for $K < 0.2$ and $K > 0.25$, up to a few times 10^{-3} in the vicinity K_c. The extrapolated data are listed in the Appendix.

III. SCALING AND LEAST-SQUARES ANALYSIS

A. Derivation from renormalization theory

The analysis of the extrapolated data was done on the basis of scaling as derived from renormalization theory. The relevant equations follow from the assumptions that the picture described in the following paragraph is valid.

The free energy density $f(T_1, T_2, \cdots)$ of the infinite system, expressed as a function of thermodynamic parameters T_j ($j = 1,\ 2,\ \cdots$), can be written as the sum of an analytic part $f_a(T_1, T_2, \cdots)$ and a singular part f_s. The singular part can be written $f_s(t_1, t_2, \cdots)$ as a function of Wegner's [22] nonlinear scaling fields t_j, which are analytic functions of the T_j in a neighborhood of a critical point under investigation. Thus

$$f(T_1, T_2, \cdots) = f_a(T_1, T_2, \cdots) + f_s(t_1, t_2, \cdots) \tag{8}$$

The singular part satisfies the scaling equation as implied by the renormalization theory. A rescaling of the linear dimensions by a factor b thus leads to

$$f_s(t_1, t_2, \cdots) = b^{-d} f_s(b^{y_1} t_1, b^{y_2} t_2, \cdots) \tag{9}$$

where d is the dimensionality and the y_j are the renormalization exponents associated with the scaling fields t_j, with the temperature exponent y_1 positive, and the other exponents negative. The choice $b = |t_1|^{-1/y_1}$ thus yields

$$f_s(t_1, t_2, \cdots) = |t_1|^{d/y_1} f_s(\pm 1, |t_1|^{-y_2/y_1} t_2, \cdots) \tag{10}$$

where ± 1 has the sign of t_1. Furthermore, $f_s(x_1, x_2, x_3, \cdots)$ is an analytic function in a neighborhood of the $x_1 = 1$, $x_2 = 0$, $x_3 = 0$, $\cdots$.

On the basis of this set of assumptions, we may Taylor expand the free energy in powers of the arguments T_j and t_j, and then expand the t_j's in the T_j's, resulting in an expression depending only on the physical temperature fields, but with expansion coefficients that remain to be determined. We follow this procedure, restricting number of scaling fields in the expansion of Eq. (10) to two, namely the temperature field $t \equiv t_1$ and the irrelevant field $\tilde{u} \equiv t_2$. The corresponding exponents are denoted y_t and y_u respectively. The temperature exponent y_t determines the leading singularity in the temperature-induced ordering

transition, while the irrelevant exponent y_u generates Wegner's correction to scaling [18]. Expansion of the right-hand side of Eq. (10) thus yields

$$f_s(t,\tilde{u}) = |t|^{d/y_t} \sum_j (j!)^{-1} f_s^{0,j}(\pm 1, 0) |t|^{-jy_u/y_t} \tilde{u}^j \,, \tag{11}$$

where $f_s^{0,j}$ is the jth derivative of f_s to its second argument. The scaling fields are expanded as analytic power series in the temperature-like parameter t_0, defined by

$$t_0 \equiv \Delta K/K \,, \qquad \Delta K \equiv K - K_{\rm c} \,. \tag{12}$$

The analytic part of the free energy f_a can be expanded directly in powers of ΔK. The resulting expansion of the total free energy density in powers of ΔK and t can be expressed in K, the only variable physical temperature parameter in our problem, as given by the Hamiltonian (1). Differentiation of the resulting expansion of the free energy density to K yields the dimensionless energy E/J. For $d = 3$ dimensions, the leading terms are included in

$$\begin{aligned} -E(K,\infty)/J = \\ \sum_{j=0,1,\cdots} e_j (\Delta K)^j + \frac{d|t|}{dK} \, a_\pm |t|^{(3-y_t)/y_t} + b_\pm u |t|^{(3-y_t-y_u)/y_t} + p_\pm u^2 |t|^{(3-y_t-2y_u)/y_t} + \cdots \,. \end{aligned} \tag{13}$$

where we have included the first three terms in the sum on j in Eq. (11), and u is an analytic function of t_0 related to $\tilde{u}$ by

$$\frac{d-y_u}{y_t} \, f_s^{0,1}(\pm 1, 0) \, \frac{d|t|}{dK} \, \tilde{u} = b_\pm u \tag{14}$$

The dimensionless specific heat C/k of the model (1) satisfies

$$\frac{C(K,\infty)}{k} = K^2 \, \frac{d^2 f(K,\infty)}{dK^2} = -\frac{K^2}{J} \, \frac{dE}{dK} \tag{15}$$

and its expansion thus follows by differentiation of the energy, Eq. (13). This leads to

$$\begin{aligned} \frac{C(K,\infty)}{kK^2} = \sum_{j=1,2,\cdots} j e_j (\Delta K)^{j-1} + \frac{3-y_t}{y_t} \left(\frac{d|t|}{dK} \right)^2 a_\pm |t|^{(3-2y_t)/y_t} + \frac{d^2|t|}{dK^2} \, a_\pm |t|^{(3-y_t)/y_t} + \\ \frac{3-y_t-y_u}{y_t} \, \frac{d|t|}{dK} \, u b_\pm |t|^{(3-2y_t-y_u)/y_t} + \frac{du}{dK} \, b_\pm |t|^{(3-y_t-y_u)/y_t} + \cdots \,, \end{aligned} \tag{16}$$

The parameters t and u, and their derivatives as they appear in Eqs. (13) and (16), are expanded in powers of t_0 as

$$t = \sum_{j=1,2,\cdots} w_j t_0^j \,, \qquad \frac{d|t|}{dK} = \pm \frac{K_{\rm c}}{K^2} \sum_{j=1,2,\cdots} j w_j t_0^{j-1} \,,$$

$$\frac{d^2|t|}{dK^2} = \pm\frac{K_c}{K^2}\sum_{j=2,3,\cdots} j(j-1)w_j t_0^{j-2} \mp \frac{K_c}{K^3}\sum_{j=1,2,\cdots} j w_j t_0^{j-1}\,, \tag{17}$$

where $\pm$ stands for the sign of t, $\mp$ for its opposite, and

$$u = \sum_{j=0,1,\cdots} u_j t_0^j\,, \qquad \frac{du}{dK} = \frac{K_c}{K^2}\sum_{j=1,2,\cdots} j u_j t_0^{j-1}\,. \tag{18}$$

The scales of t and u are determined by setting $w_1 = u_0 = 1$.

B. Fits

Whereas Eq. (11) includes, in principle, infinitely many terms, for numerical work it is necessary to truncate the expansion of f_s, as well as those of f_a and the scaling fields, at a finite order. Expression (13) for the energy already contains the implicit simplification that there is only one irrelevant field, and that the expansion of $f_s(\pm 1, x)$ is truncated at second order. Moreover, higher orders in the expansion of the temperature derivative of the irrelevant field were neglected. We shall reconsider these simplifications in Sec. IV A. No further simplifications were made in the derivation of Eq. (16) from Eq. (13).

Many attempts were made to fit Eqs. (13) and (16) to the numerical data, using different ranges of K, and different sets of parameters as determined by the orders at which the expansions were truncated. The unknown parameters in each set were determined by means of a Levenberg-Marquardt nonlinear least-squares analysis. Since Eqs. (13) and (16) depend on the same parameters, the data for the energy and the heat capacity were simultaneously fitted by one set of parameters.

A fit was considered satisfactory if it met three criteria: first, the residual χ^2 has to be compatible with the number of degrees of freedom; second, there should be sufficiently large ranges of overlap with the accurate predictions from the low- and high-temperature series expansions; and third, at least the amplitudes of the leading terms in the fit formulas should be reasonably stable under variations of the K-interval and of the number of correction terms in the temperature field and the analytic background. In Table I we list the smallest satisfactory set of parameters thus obtained. We skipped the ellipses in Eqs. (13) and (16), and included terms up to order $j = 4$ in the expansion of t, up to $j = 2$ in that of u, and up to $j = 5$ in the analytic parts expressed by the first sums in Eqs. (13) and (16). The residual of this fit was $\chi^2 = 53.5$, to be compared with the number of degrees of freedom $d_f = 84$. Since

possible correlations between specific heat and energy data could influence the estimation of the errors in the fitted parameters, we have analyzed the correlations between the deviations of the energy and of the specific heat with respect to the fit formula. We find a correlation coefficient of -0.066 which is not significant, and does not provide a reason to reconsider our error estimates.

During the least-squares analysis, we found that some parameter values changed significantly when the K-interval and/or the numbers of parameters in the expansions of t and of the analytic background were varied. Such shifts were sometimes comparable to the error margins as estimated from statistics based on the accuracy of the Monte Carlo results. This applied in particular to those of the w_j and the e_j with $j > 2$. In this respect the amplitudes a_+, a_-, e_0, e_1 and, to some extent, b_+ and b_- were better behaved. The error estimates listed in Table I take into account the variation of the parameter values between these fits.

IV. DISCUSSION

A. Choice of parameters and their error margins

Equation (11) and the fits of E and C use only one irrelevant field, while, according to Newman and Riedel [23], corrections to scaling could also arise from a second irrelevant field u' with exponent $y_{u'} \approx 2y_u$. We note that corrections generated in first order of u' would thus, in the present context, be practically indistinguishable from those generated in second order by u. For this reason, we have not included a separate term containing u'. Furthermore, the energy, Eq. (13), neglects a contribution due to the possible K-dependence of the irrelevant field. Such a term behaves as $|t|^{(3-y_u)/y_t}$ and is thus a factor $|t|$ smaller than the leading correction. The third-order correction in u, which is also neglected, has nearly the same exponent.

Another correction that was neglected is one with an integer exponent $y'' = -2$, associated with the discreteness of the cubic lattice. The presence of such corrections could modify the higher-order correction amplitudes given in Table I, but the χ^2 criterion did not yield indications that a term with $y'' = -2$ should be included.

Some insight in the relative importance of the corrections due to different orders of the irrelevant field can be obtained by comparing the fit including the second order of u, as given

TABLE I: Values of the parameters in the fit according to Eqs. (13) and (16) to Monte Carlo data in the interval $0.15 \leq K \leq 0.60$. The error estimates given in the last column are not only based on statistics, but also on the variations of the parameter values due to changes of the fit interval and the number of parameters. In two cases the estimated error exceeds the parameter value and no error is quoted. While these values have no physical meaning, they are still useful for the evaluation of the specific heat and the energy. The values of y_t, y_u, and K_c were taken from Ref. 14.

parameter	value	error margin
w_1	1	fixed
w_2	0.662300	0.06
w_3	0.160415	0.09
w_4	0.008397	——
u_0	1	fixed
u_1	-2.673700	0.6
a_-	1.466642	0.016
a_+	2.758572	0.012
b_-	0.923100	0.2
b_+	-2.694381	0.4
p_-	-1.440041	0.4
p_+	-2.345305	0.8
e_0	0.990604	0.000004
e_1	-27.847250	0.8
e_2	110.506127	12
e_3	-193.032628	50
e_4	186.624090	100
e_5	-80.141986	——
y_t	1.587	fixed
y_u	-0.82	fixed
K_c	0.2216546	fixed

in Table I, to fits including up to the first order. Reasonable fits, as following from the χ^2 criterion, could only be be obtained by including three more coefficients e_j or w_j. Moreover, these coefficients tended to assume much larger values. For this reason, we prefer the fit up to second order in u, although the fit up to first order also yields a satisfactory numerical representation of the critical energy and specific heat.

Only the parameters a_-, a_+, c_0 and c_1, describing the leading few orders of E and C, were about the same for both types of fits. It is thus clear that not too much physical significance should be given to the subleading and higher-order parameters given in Table I, except that they provide a numerical description of E and C in the critical region.

The relative errors in the amplitudes p_- and p_+ of the second order term in u, as given in Table I, are appreciable, and far exceed those of the first-order amplitudes b_- and b_+. For this reason we believe that it is not necessary to include a third-order correction, or other terms with approximately the same exponent.

B. Comparison with existing results

1. Series expansions

Numerical evaluation of Eq. (16) allows comparison with results from series expansions. The low-temperature series for the energy is provided by Bhanot et al. [15] up to order 25 in e^{-2K}. The specific heat, as obtained by differentiation of this series, is in good agreement with Eq. (16) in the interval $0.39 < K < 0.60$. The differences, which are shown in Fig. 1, do not exceed 10^{-4}. For $K > 0.60$, outside the range of the least-squares fit, our representation of the specific heat with Eq. (16) is no longer accurate and the differences increase sharply. The increasing differences for $K < 0.30$ are due to the truncation of the low-temperature series to 25 terms.

For temperatures above the critical point, a comparison can be made based on the series expansion up to order 46 of the free energy as provided by Arisue and Fujiwara [16], with the help of Eq. (3). The differences with Eq. (16) are less than 10^{-4} interval $0.15 < K < 0.19$, as plotted in Fig. 2. For $K < 0.15$, outside the range of the fit, Eq. (16) rapidly loses its accuracy. The increasing differences for $K > 0.19$ are due to the truncation of the series.

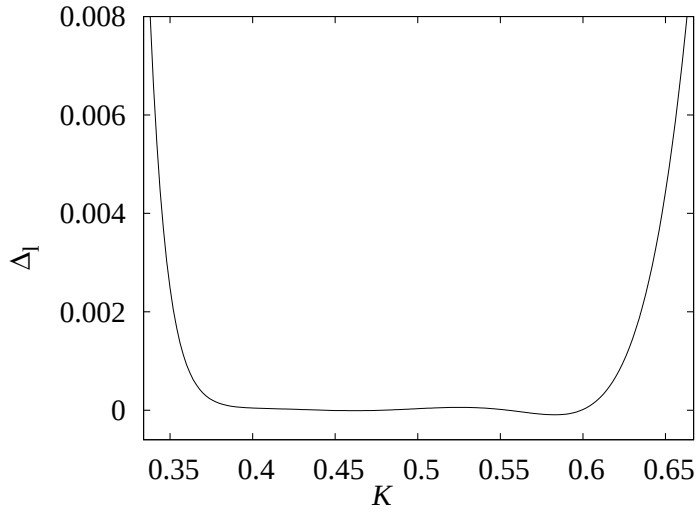

FIG. 1: Difference $\Delta_{\rm l} \equiv (C_{\rm LTE} - C_{\rm fit})/k$ between the specific heat of the Ising model as obtained from the low-temperature series of the energy and from the present least-squares analysis according to Eq. (16). The difference $\Delta_{\rm l}$ is at most 10^{-4} in the interval $0.39 < K < 0.60$.

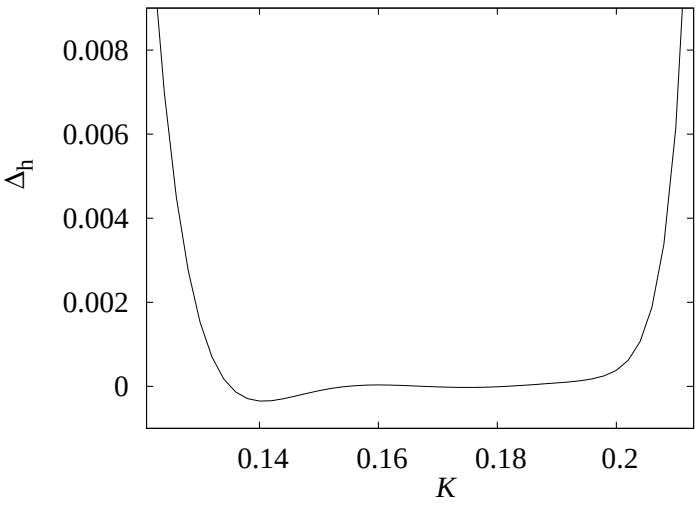

FIG. 2: Difference $\Delta_{\rm h} \equiv (C_{\rm HTE} - C_{\rm fit})/k$ between the specific heat of the Ising model as obtained from the high-temperature series of the energy and from the present least-squares analysis according to Eq. (16). The difference $\Delta_{\rm h}$ is at most 10^{-4} in the interval $0.15 < K < 0.19$.

2. Amplitude ratios and analytic background

The fit up to first order in u yielded a universal amplitude ratio $a_-/a_+ = 0.540$ (5), which is to be compared to the result of the fit including the second order of u, which is

$a_-/a_+ = 0.532$ (7) as follows from the parameter values in Table I. Based on the consistency between these two results, we believe that the latter result $a_-/a_+ = 0.532$ (7) is reliable. This result is close to an estimate 0.541 (14) by Bagnuls et al. [24] from field theory, and to the result 0.523 (9) obtained by Liu and Fisher [25] based on series expansions, and slightly smaller than 0.560 (10) as determined from Monte Carlo data by Hasenbusch and Pinn [26].

Another universal ratio that can be constructed from the results in Table I concerns the corrections-to-scaling amplitudes. The data in the table suggest $b_-/b_+ = -0.34$ (9), which differs considerably from $b_-/b_+ = -0.96$ (25) as obtained by Bagnuls et al. [24] (note the sign difference with respect to the notation used by Bagnuls et al., which is related to the factor $d|t|/dK$ in our Eq. (16)). The sign of this amplitude ratio is in agreement with the conclusions of Liu and Fisher [27].

As noted in Sec. IV A, there may be corrections to scaling governed by an irrelevant field u' with exponent $y_{u'} \approx 2y_u$, and thus indistinguishable from contributions in second order of u. It is thus possible that the amplitudes p_+ and p_- as given in Table I contain contributions due to the field u'. Therefore, the resulting ratio $p_-/p_+ = 0.61$ (24) may not qualify as a universal amplitude ratio.

Our result for the critical energy, $e_0 = 0.990604$ (4), can be compared with results obtained from series analysis. It is slightly smaller than the result $e_0 = 0.99218$ (15) obtained by Sykes et al. [28], slightly larger than $e_0 = 0.9902$ (1) found by Liu and Fisher [25], and in agreement with $e_0 = 0.991$ (1) found by Butera and Comi [29]. Our result is also consistent with the Monte Carlo estimates $e_0 = 0.990$ (4) due to Jensen and Mouritsen [30], and $e_0 = 0.9904$ (8) due to Hasenbusch and Pinn [26].

3. Comparison with experimental results for Rb_3CoCl_5

As implied in the Introduction, the magnetic Co^{2+} ions in rubidium cobalt chloride assume a spin-1/2 Ising character. This has been experimentally confirmed [31] in the related compound Cs_3CoCl_5. The magnetic moments are aligned along the c direction of the tetragonal crystal structure. The Co^{2+} ions are arranged in a simple Bravais lattice, with equivalent positions [32]. Furthermore, electron-spin resonance results [33] for Cs_3CoCl_5 showed that the exchange interaction with the two nearest neighbors in the crystallographic c direction has the same magnitude as that with the four nearest neighbors in the aa plane,

so that one may expect that the theoretical results for the simple-cubic Ising model are applicable. Specific-heat and magnetic susceptibility measurements [9] on Rb_3CoCl_5 showed that a phase transition to an antiferromagnetic phase occurs at $T_c = 1.14$ K. It was indeed found that the specific heat (which does not depend on the sign of K) did agree with the theoretical predictions available at that time. These predictions were based on series expansions due to Baker [34] and Sykes [35], and on the assumption that the specific-heat exponent $\alpha = 0$. In view of later results for the specific-heat exponent, as well as the effect of Wegner's correction [18], the comparison made in Ref. 9 may thus not be considered as entirely satisfactory. In Fig. 3 we show the experimental data together with Eq. (16), as well as results from the low- and high-temperature series. This comparison with the experimental data, which involves only one adjustable parameter, the critical temperature, shows that the specific heat of Rb_3CoCl_5 agrees reasonably well with the predictions for the simple-cubic Ising model. The data in Fig. 3 suggest small deviations at low as well as at high temperatures, but there the specific heat becomes very small, so that the experimental error margins, which include the uncertainty of heat capacity of the empty apparatus, become appreciable. A comparison of the experimental data listed in Ref. 9 with the results from Eq. (16) show that deviations up to a few percent occur also in the range $0.9 < K/K_c < 1.2$. But these deviations do not display an obvious systematical trend, and may possibly be attributed to the fact that the measured heat capacity is, near criticality, the result of integration of a highly nonlinear function over a nonzero temperature range.

It thus seems that new experiments on Rb_3CoCl_5 are needed to firmly establish deviations with respect to the predictions for the simple-cubic Ising model. Such deviations would be a logical consequence of the tetragonal symmetry of Rb_3CoCl_5, which implies that there is no reason why the coupling in the c-direction should be precisely equal to that in the a direction. Also the presence of interactions with further neighbor spins, which include small magnetic dipole-dipole interactions, should lead to deviations.

C. Conclusion

The formula Eq. (16), supplemented by Eqs. (17), (18), and (12) and by the parameter values in Table I, describes the specific heat of the three-dimensional Ising model in the interval $0.15 < J/kT < 0.60$. Comparisons with low- and high-temperature series expansions

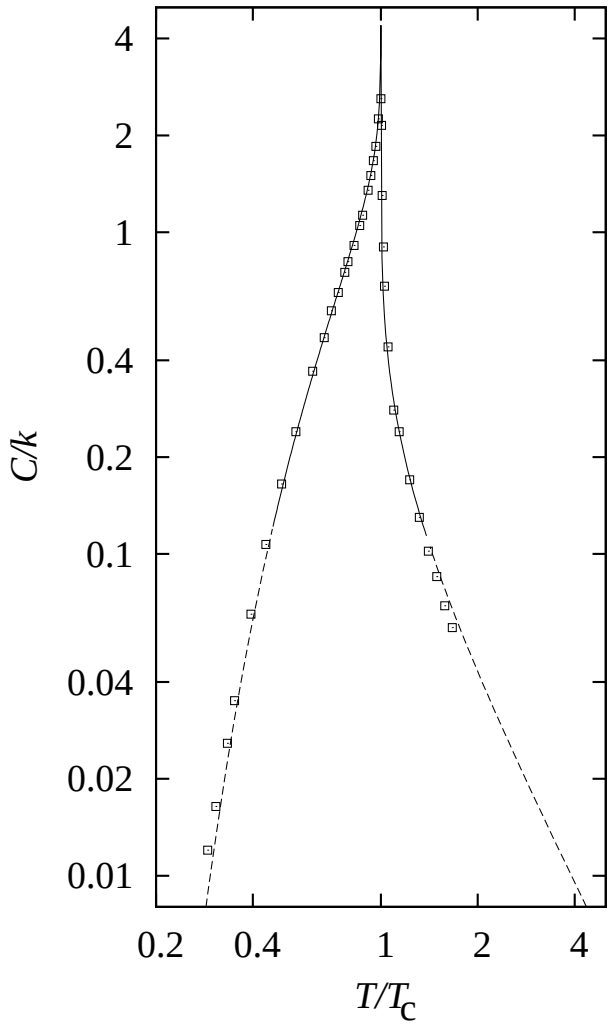

FIG. 3: Specific heat of the Ising model on the simple-cubic lattice. Logarithmic scales are used because of the large variation of the specific heat with temperature. The data points are existing experimental results [9] for Rb_3CoCl_5. The full line represents the scaling form Eq. (16) with the parameters defined in Table I. The dashed lines at the lower left and right are obtained from low- and high-temperature series expansions [15, 16] of the the free energy.

yield satisfactory agreement in the intervals $0.15 < J/kT < 0.19$ and $0.39 < J/kT < 0.60$ respectively. The differences between Eq. (16) and the results from series expansions are at most 10^{-4} in the mentioned intervals. These differences are smaller than the statistical errors in the Monte Carlo results on which Table I is based, as may be expected since the number of 100 data points far exceeds the number of 16 free parameters in the fit formula, so that in effect averaging occurs. Since Eq. (16) continues to satisfactorily describe the

extrapolated Monte Carlo data until a distance $|K - K_c| \approx 0.005$ from the critical point, we conclude that the error margin in Eq. (16) does not exceed that of the Monte Carlo data, i.e., it will be limited to at most a few times 10^{-3} at $|K - K_c| > 0.005$. Larger uncertainties are expected for $|K - K_c| < 0.005$ because of the error margins in the critical amplitudes, exponents and temperature. Taking into account these numerical uncertainties, Eq. (16) can be used in the interval $0.15 < J/kT < 0.60$ for comparison with experiments on systems that are described by the simple-cubic Ising Hamiltonian.

In addition, our results show that Monte Carlo simulations can be used to determine the universal leading amplitude ratios a_-/a_+ and even the nonasymptotic ratio b_-/b_+. Thus far, the correction amplitudes have been studied by means of series analysis, field theory, and crossover scaling, see e.g., Refs. 24, 27, 36, 37.

Acknowledgments

HB thanks J.M.J. van Leeuwen for valuable discussions, and the Lorentz Fund (The Netherlands) for financial support.

---

[1] E. Ising, Z. Physik **31**, 253 (1925).

[2] M. Suzuki, Phys. Lett. A **35**, 23 (1971); M. Suzuki and F. Tanaka, Prog. Theor. Phys. **3**, 1085 (1973).

[3] M. E. Fisher and P. Pfeuty, Phys. Rev. B **6**, 1889 (1972).

[4] F. J. Wegner, Phys. Rev. B **6**, 1891 (1972).

[5] L. J. de Jongh and A. R. Miedema, Adv. Phys. **23**, 1 (1974).

[6] W. P. Wolf, Braz. J. of Phys. [online] **30**, n. 4, 794 (2000).

[7] J. C. Wright, H. W. Moos, J. H. Colwell, B. W. Magnum and D. D. Thornton, Phys. Rev. B **3**, 843 (1971).

[8] R. F. Wielinga, H. W. J. Blöte, J. A. Roest and W. J. Huiskamp, Physica (Amsterdam) **34** 223 (1967).

[9] H. W. J. Blöte and W. J. Huiskamp, Phys. Lett. A **29**, 304 (1969).

[10] Z.-D. Zhang, Phil. Mag. **87**, 5309 (2008).

[11] J. H. H. Perk, arXiv:0811.1802.v2 (2008).

[12] F. Y. Wu, B. M. McCoy, M. E. Fisher and L. Chayes, Phil. Mag. **88**, 3093 (2008).

[13] P. Butera and M. Comi, Phys. Rev. B **62**, 14837 (2004).

[14] Y. Deng and H. W. J. Blöte, Phys. Rev. E **68**, 036125 (2003), and references therein.

[15] G. Bhanot, M. Creutz and J. Lacki, Phys. Rev. Lett. **69**, 1841 (1992); G. Bhanot, M. Creutz, U. Glassner and K. Schilling, Phys. Rev. B **49**, 12909 (1994).

[16] H. Arisue and T. Fujiwara, Phys. Rev. E **67**, 066109 (2003). There is a typo in the 42th order term; the correct value appears in hep-lat/0209002 (2002).

[17] P. Butera and M. Comi, Phys. Rev. B **69**, 174416 (2004).

[18] F. J. Wegner, Phys. Rev. B **5**, 4529 (1972).

[19] R. H. Swendsen and J. S. Wang, Phys. Rev. Lett. **58**, 86 (1987).

[20] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).

[21] For reviews, see e.g. M. P. Nightingale in *Finite-Size Scaling and Numerical Simulation of Statistical Systems*, ed. V. Privman (World Scientific, Singapore 1990), and M. N. Barber in *Phase Transitions and Critical Phenomena*, eds. C. Domb and J. L. Lebowitz (Academic, New York 1983), Vol. 8.

[22] F. J. Wegner, in *Phase Transitions and Critical Phenomena*, eds. C. Domb and M. S. Green (Academic, N.Y. 1976), Vol. 6.

[23] K. E. Newman and E. K. Riedel, Phys. Rev. B bf 30, 6615 (1984).

[24] C. Bagnuls, C. Bervillier, D. I. Meiron and B. G. Nickel, Phys. Rev. B **35**, 3585 (1987).

[25] A. J. Liu and M. E. Fisher, Physica A (Amsterdam) **156**, 35 (1989).

[26] M. Hasenbusch and A. Pinn, J. Phys. A **31**, 6157 (1998).

[27] A. Liu and M. E. Fisher, J. Stat. Phys. **58**, 431 (1990).

[28] M. F. Sykes, D. L. Hunter, D. S. McKenzie and B. R. Heap, J. Phys. A **5**, 667 (1972).

[29] P. Butera and M. Comi, Phys. Rev. B **60**, 6749 (1999).

[30] S. J. K. Jensen and O. G. Mouritsen, J. Phys. A **15**, 2631 (1982).

[31] H. G. Beljers, P. F. Bongers, R. P. van Stapele and H. Zijlstra, Phys. Letters **12**, 81 (1964).

[32] H. M. Powell and A. F. Wells, J. Chem. Soc. 359 (1935).

[33] R. P. van Stapele, J. C. M. Henning, G. E. G. Hardeman and P. F. Bongers, Phys. Rev. **150**, 310 (1966).

[34] J. M. Baker. Phys. Rev. **129**, 99 (1963).

[35] M. F. Sykes, private communication cited in Ref. 9.

[36] R. Schloms and V. Dohm, Phys. Rev. B **42**, 6142 (1990).

[37] M. A. Anisimov, S. B. Kiselev, J. V. Sengers and S. Tang, Physica A (Amsterdam) **188**, 487 (1992).

APPENDIX: EXTRAPOLATED ENERGY AND SPECIFIC HEAT

TABLE II: Extrapolated values of the dimensionless energy density of the infinite, simple-cubic Ising model as a function of the coupling K. Estimated error bounds are included.

K	$-E(K)$	error	K	$-E(K)$	error
0.12	0.382236	0.000020	0.13	0.419100	0.000109
0.14	0.457696	0.000007	0.15	0.498271	0.000098
0.16	0.541261	0.000008	0.166	0.568535	0.000448
0.17	0.587433	0.000007	0.172	0.597108	0.000047
0.178	0.627251	0.000049	0.18	0.637719	0.000009
0.184	0.659300	0.000052	0.19	0.693640	0.000008
0.195	0.724504	0.000007	0.196	0.730987	0.000060
0.2	0.757945	0.000005	0.202	0.77224	0.000011
0.205	0.794807	0.000016	0.21	0.836533	0.000053
0.213	0.865007	0.002836	0.22165460	0.990604	0.000004
0.224	1.135886	0.000083	0.225	1.184077	0.000113
0.226	1.228851	0.002835	0.227	1.270902	0.001567
0.228	1.310761	0.000069	0.229	1.348806	0.000084
0.23	1.385036	0.000010	0.232	1.453408	0.000128
0.235	1.547095	0.000082	0.24	1.684411	0.000006
0.25	1.908377	0.000006	0.26	2.084422	0.000011
0.268	2.200165	0.000117	0.27	2.226207	0.000025
0.28	2.342331	0.000013	0.29	2.438392	0.000020
0.3	2.518570	0.000013	0.31	2.585908	0.000017
0.32	2.643039	0.000137	0.33	2.691193	0.000121
0.34	2.732442	0.000779	0.35	2.767639	0.000008
0.36	2.797886	0.000224	0.37	2.823926	0.000119
0.38	2.846340	0.000055	0.39	2.865798	0.000070
0.4	2.882622	0.000005	0.42	2.909917	0.000030
0.44	2.930623	0.000034	0.45	2.939050	0.000003
0.46	2.946380	0.000022	0.48	2.958427	0.000035
0.5	2.967777	0.000002	0.6	2.990703	0.000001
0.65	2.994958	0.000001	0.7	2.997255	0.000001

TABLE III: Extrapolated values of the dimensionless specific heat of the infinite, simple-cubic Ising model as a function of the coupling K. Estimated error bounds are included.

K	$C(K)/k$	error	K	$C(K)/k$	error
0.12	0.05212	0.00004	0.14	0.07736	0.00005
0.15	0.09382	0.00013	0.16	0.11381	0.00004
0.166	0.12812	0.00008	0.17	0.13882	0.00005
0.172	0.14458	0.00010	0.178	0.16391	0.00012
0.18	0.17094	0.00012	0.19	0.21445	0.00035
0.195	0.24361	0.00031	0.2	0.27950	0.00110
0.205	0.32850	0.00093	0.208	0.36500	0.00100
0.21	0.39573	0.00114	0.214	0.48216	0.00165
0.215	0.51335	0.00261	0.216	0.54767	0.00157
0.217	0.58500	0.00200	0.227	2.11009	0.00675
0.228	2.01738	0.00323	0.229	1.95000	0.01000
0.23	1.87829	0.00300	0.232	1.76800	0.00150
0.235	1.64500	0.01000	0.238	1.52800	0.00300
0.24	1.46600	0.00200	0.25	1.23138	0.00041
0.26	1.06294	0.00031	0.27	0.93268	0.00200
0.28	0.82520	0.00060	0.29	0.73597	0.00094
0.3	0.66021	0.00072	0.31	0.59383	0.00085
0.35	0.39923	0.00039	0.36	0.36325	0.00036
0.37	0.33045	0.00024	0.38	0.30110	0.00020
0.39	0.27460	0.00020	0.4	0.25058	0.00025
0.42	0.20890	0.00020	0.44	0.17428	0.00013
0.45	0.15910	0.00020	0.46	0.14567	0.00012
0.48	0.12158	0.00010	0.5	0.10160	0.00010
0.55	0.06470	0.00015	0.6	0.04109	0.00010
0.65	0.02593	0.00008	0.7	0.01632	0.00004